



Full wwPDB NMR Structure Validation Report ⓘ

Sep 27, 2022 – 11:08 am BST

PDB ID : 7P55
BMRB ID : 34650
Title : NMR structure of human ACE2 21-42 fragment in HFIP/water 50/50 v/v
Authors : Santoro, A.; Buonocore, M.; Grimaldi, M.; D'Ursi, A.M.
Deposited on : 2021-07-14

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.31.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

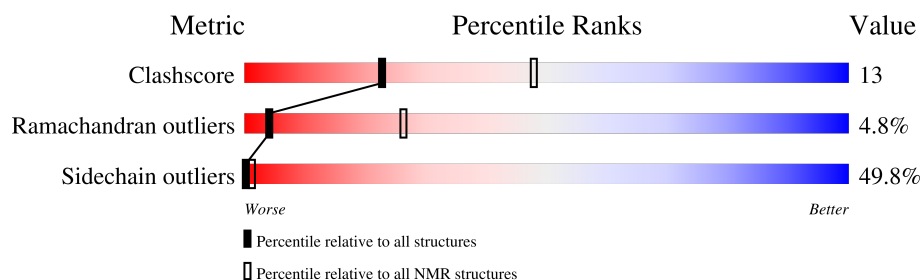
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 63%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	22	

2 Ensemble composition and analysis

This entry contains 50 models. Model 41 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:22-A:42 (21)	0.09	41

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 5 single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 17, 19, 20, 21
2	30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47
3	23, 24, 25, 26, 27
4	1, 2, 18
5	28, 29
Single-model clusters	16; 22; 48; 49; 50

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 365 atoms, of which 173 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Processed angiotensin-converting enzyme 2.

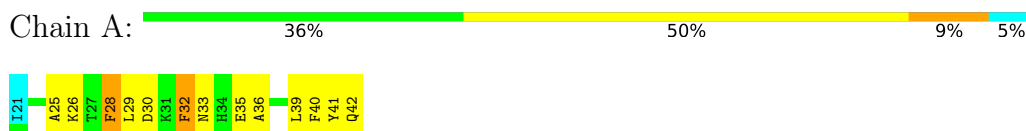
Mol	Chain	Residues	Atoms					Trace
1	A	22	Total	C	H	N	O	0
			365	124	173	29	39	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Processed angiotensin-converting enzyme 2

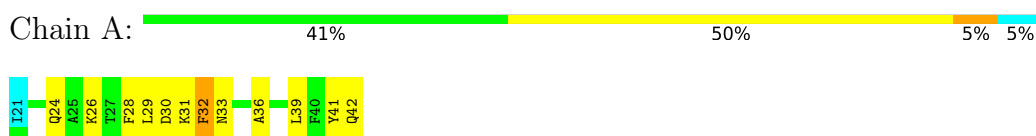


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

- Molecule 1: Processed angiotensin-converting enzyme 2



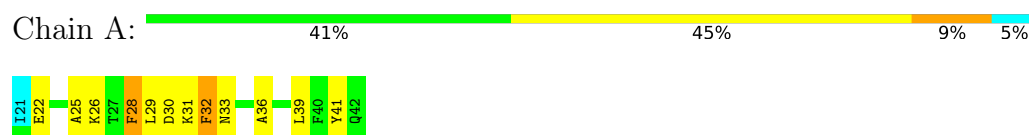
4.2.2 Score per residue for model 2

- Molecule 1: Processed angiotensin-converting enzyme 2



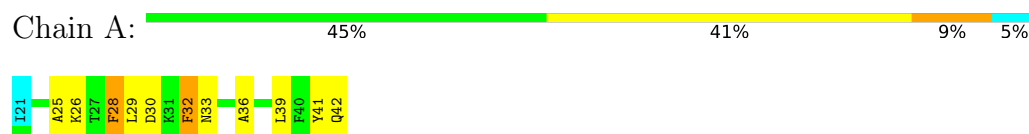
4.2.3 Score per residue for model 3

- Molecule 1: Processed angiotensin-converting enzyme 2



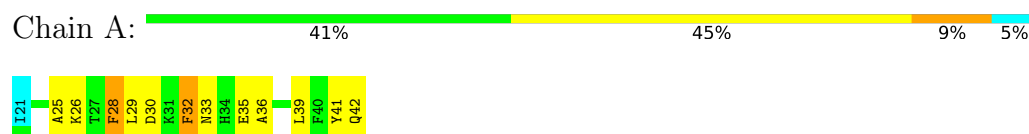
4.2.4 Score per residue for model 4

- Molecule 1: Processed angiotensin-converting enzyme 2



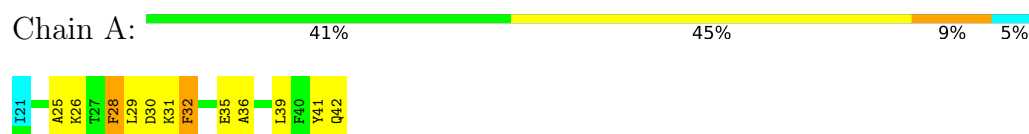
4.2.5 Score per residue for model 5

- Molecule 1: Processed angiotensin-converting enzyme 2



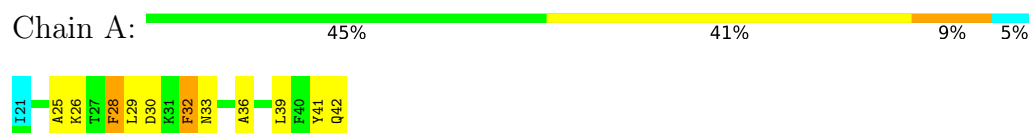
4.2.6 Score per residue for model 6

- Molecule 1: Processed angiotensin-converting enzyme 2



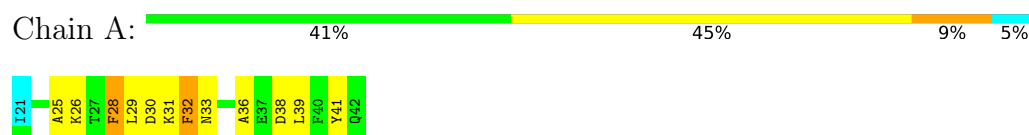
4.2.7 Score per residue for model 7

- Molecule 1: Processed angiotensin-converting enzyme 2



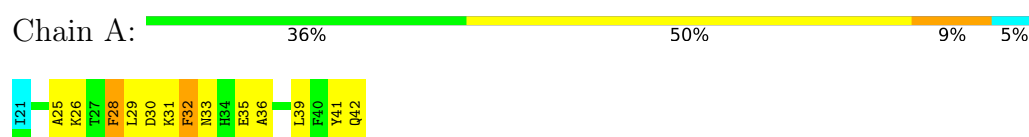
4.2.8 Score per residue for model 8

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.9 Score per residue for model 9

- Molecule 1: Processed angiotensin-converting enzyme 2



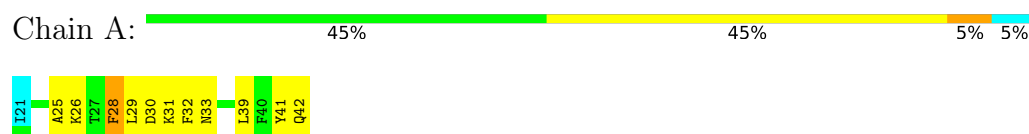
4.2.10 Score per residue for model 10

- Molecule 1: Processed angiotensin-converting enzyme 2



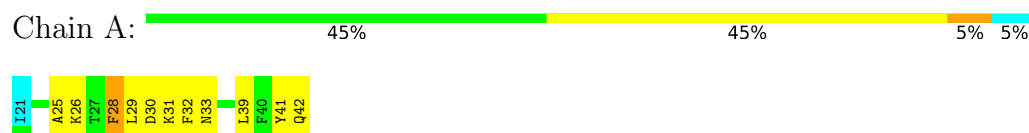
4.2.11 Score per residue for model 11

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.12 Score per residue for model 12

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.13 Score per residue for model 13

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.14 Score per residue for model 14

- Molecule 1: Processed angiotensin-converting enzyme 2



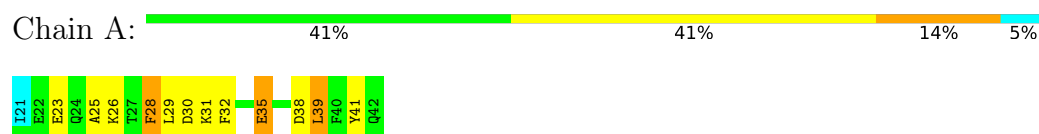
4.2.15 Score per residue for model 15

- Molecule 1: Processed angiotensin-converting enzyme 2



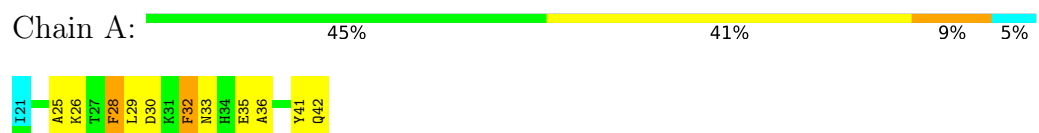
4.2.16 Score per residue for model 16

- Molecule 1: Processed angiotensin-converting enzyme 2



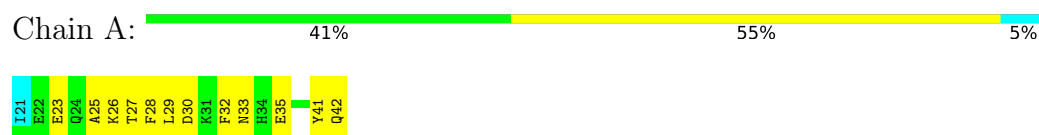
4.2.17 Score per residue for model 17

- Molecule 1: Processed angiotensin-converting enzyme 2



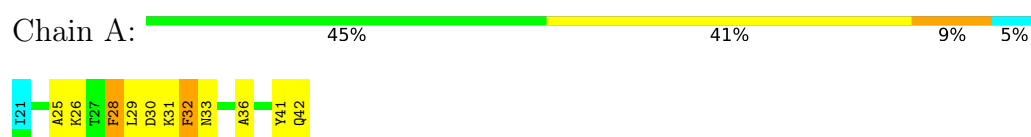
4.2.18 Score per residue for model 18

- Molecule 1: Processed angiotensin-converting enzyme 2



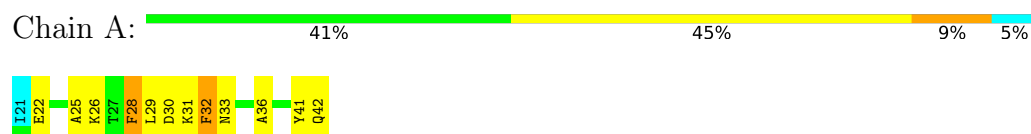
4.2.19 Score per residue for model 19

- Molecule 1: Processed angiotensin-converting enzyme 2



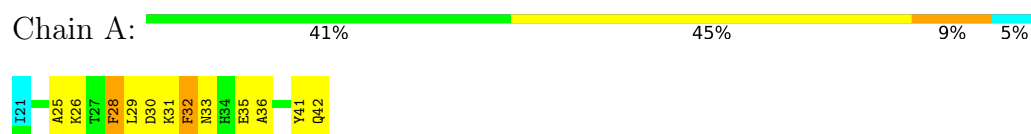
4.2.20 Score per residue for model 20

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.21 Score per residue for model 21

- Molecule 1: Processed angiotensin-converting enzyme 2



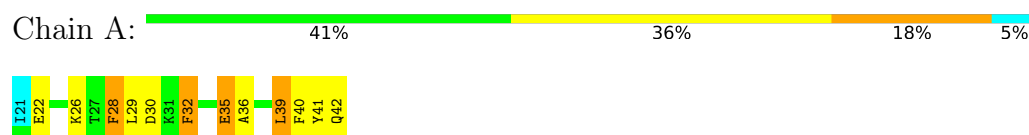
4.2.22 Score per residue for model 22

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.23 Score per residue for model 23

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.24 Score per residue for model 24

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.25 Score per residue for model 25

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.26 Score per residue for model 26

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.27 Score per residue for model 27

- Molecule 1: Processed angiotensin-converting enzyme 2



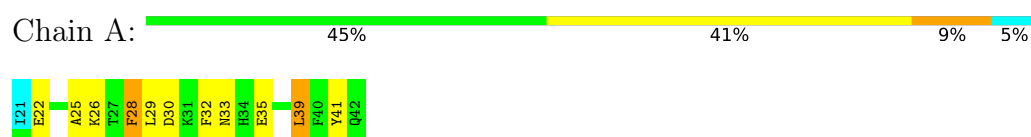
4.2.28 Score per residue for model 28

- Molecule 1: Processed angiotensin-converting enzyme 2



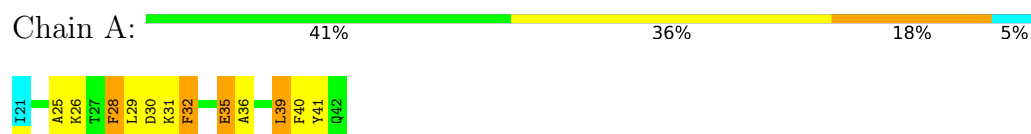
4.2.29 Score per residue for model 29

- Molecule 1: Processed angiotensin-converting enzyme 2



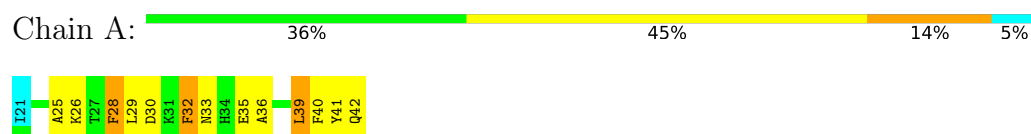
4.2.30 Score per residue for model 30

- Molecule 1: Processed angiotensin-converting enzyme 2



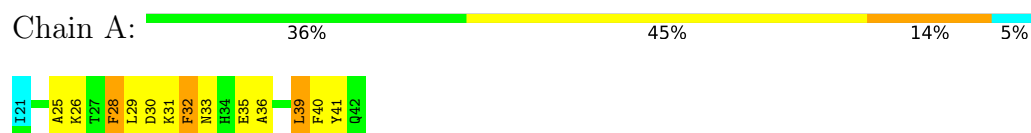
4.2.31 Score per residue for model 31

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.32 Score per residue for model 32

- Molecule 1: Processed angiotensin-converting enzyme 2



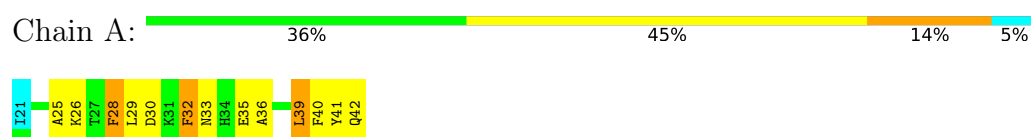
4.2.33 Score per residue for model 33

- Molecule 1: Processed angiotensin-converting enzyme 2



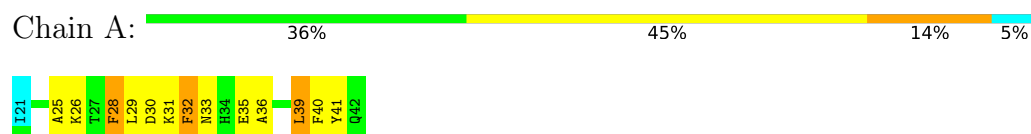
4.2.34 Score per residue for model 34

- Molecule 1: Processed angiotensin-converting enzyme 2



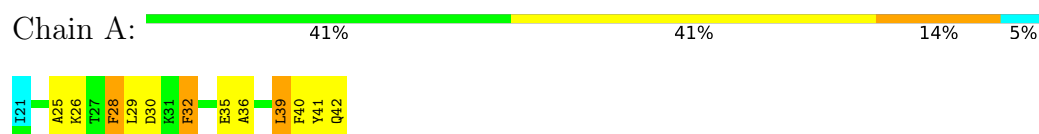
4.2.35 Score per residue for model 35

- Molecule 1: Processed angiotensin-converting enzyme 2



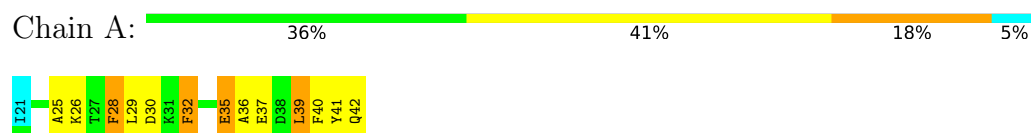
4.2.36 Score per residue for model 36

- Molecule 1: Processed angiotensin-converting enzyme 2



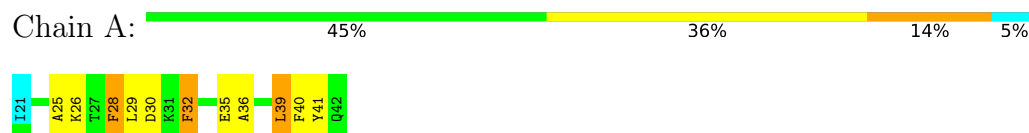
4.2.37 Score per residue for model 37

- Molecule 1: Processed angiotensin-converting enzyme 2



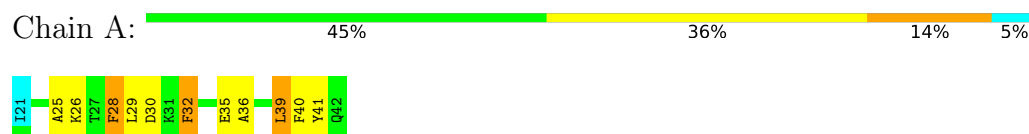
4.2.38 Score per residue for model 38

- Molecule 1: Processed angiotensin-converting enzyme 2



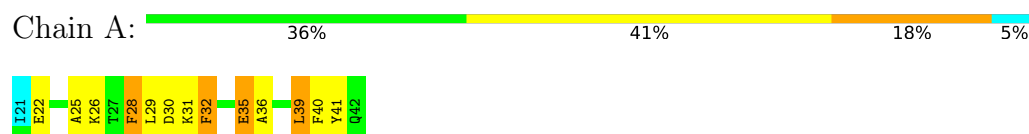
4.2.39 Score per residue for model 39

- Molecule 1: Processed angiotensin-converting enzyme 2



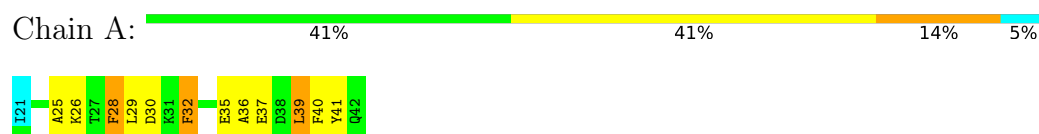
4.2.40 Score per residue for model 40

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.41 Score per residue for model 41 (medoid)

- Molecule 1: Processed angiotensin-converting enzyme 2



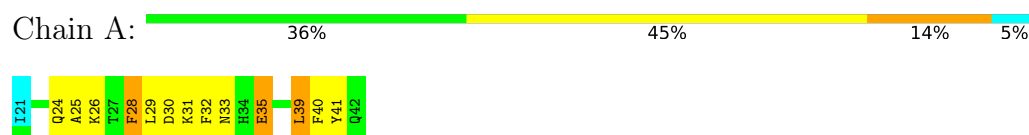
4.2.42 Score per residue for model 42

- Molecule 1: Processed angiotensin-converting enzyme 2



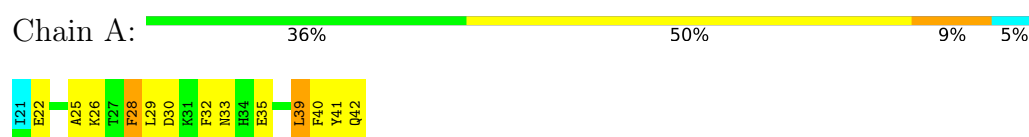
4.2.43 Score per residue for model 43

- Molecule 1: Processed angiotensin-converting enzyme 2



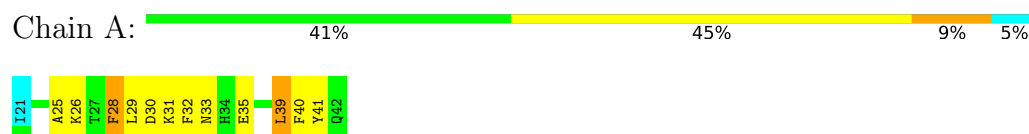
4.2.44 Score per residue for model 44

- Molecule 1: Processed angiotensin-converting enzyme 2



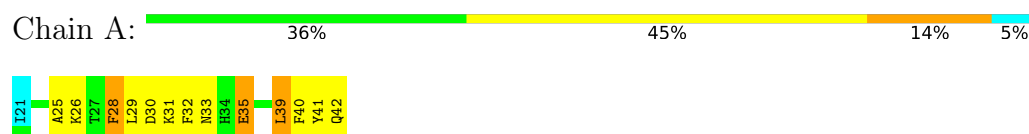
4.2.45 Score per residue for model 45

- Molecule 1: Processed angiotensin-converting enzyme 2



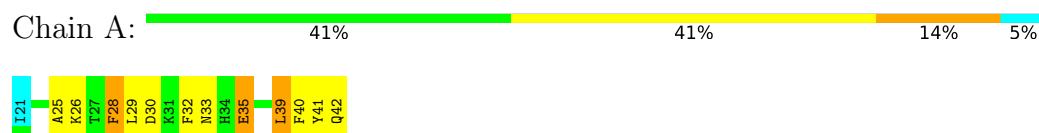
4.2.46 Score per residue for model 46

- Molecule 1: Processed angiotensin-converting enzyme 2



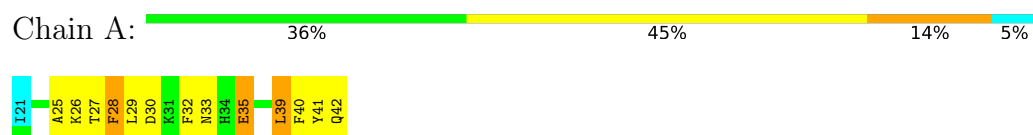
4.2.47 Score per residue for model 47

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.48 Score per residue for model 48

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.49 Score per residue for model 49

- Molecule 1: Processed angiotensin-converting enzyme 2



4.2.50 Score per residue for model 50

- Molecule 1: Processed angiotensin-converting enzyme 2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 50 calculated structures, 50 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
TALOS-N	refinement	
CYANA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	202
Number of shifts mapped to atoms	202
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	63%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	184	162	162	4±3
All	All	9200	8100	8100	217

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HD13	1:A:40:PHE:N	0.86	1.85	50	25
1:A:39:LEU:O	1:A:39:LEU:HD22	0.78	1.79	34	25
1:A:39:LEU:HD13	1:A:39:LEU:C	0.62	2.14	50	25
1:A:35:GLU:CD	1:A:39:LEU:HD13	0.59	2.18	16	1
1:A:39:LEU:HD22	1:A:39:LEU:C	0.55	2.22	25	25
1:A:35:GLU:OE1	1:A:39:LEU:HD13	0.53	2.02	16	1
1:A:35:GLU:HG3	1:A:39:LEU:HD23	0.52	1.82	28	2
1:A:39:LEU:O	1:A:39:LEU:HD12	0.51	2.05	29	2
1:A:39:LEU:HD12	1:A:39:LEU:C	0.51	2.26	29	2
1:A:35:GLU:O	1:A:39:LEU:HD12	0.50	2.07	50	25
1:A:39:LEU:C	1:A:39:LEU:CD1	0.45	2.84	50	1
1:A:23:GLU:HA	1:A:27:THR:HG22	0.45	1.88	18	6
1:A:34:HIS:CG	1:A:35:GLU:N	0.45	2.82	49	2
1:A:32:PHE:O	1:A:36:ALA:HB2	0.45	2.11	21	30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:HIS:ND1	1:A:35:GLU:N	0.43	2.66	50	1
1:A:28:PHE:O	1:A:28:PHE:CD1	0.42	2.73	16	43
1:A:39:LEU:C	1:A:39:LEU:CD2	0.40	2.90	32	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	20/22 (91%)	18±1 (89±4%)	1±1 (6±4%)	1±0 (5±1%)	4	26
All	All	1000/1100 (91%)	895 (90%)	57 (6%)	48 (5%)	4	26

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	25	ALA	48

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	19/20 (95%)	10±1 (50±6%)	9±1 (50±6%)	0	1
All	All	950/1000 (95%)	477 (50%)	473 (50%)	0	1

All 18 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	26	LYS	50
1	A	28	PHE	50

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Mol	Chain	Res	Type	Models (Total)
1	A	29	LEU	50
1	A	30	ASP	50
1	A	41	TYR	50
1	A	32	PHE	49
1	A	39	LEU	44
1	A	33	ASN	35
1	A	42	GLN	32
1	A	31	LYS	24
1	A	35	GLU	16
1	A	22	GLU	7
1	A	38	ASP	4
1	A	24	GLN	3
1	A	37	GLU	3
1	A	23	GLU	2
1	A	27	THR	2
1	A	34	HIS	2

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 63% for the well-defined parts and 63% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	202
Number of shifts mapped to atoms	202
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 63%, i.e. 175 atoms were assigned a chemical shift out of a possible 277. 2 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	57/105 (54%)	42/42 (100%)	15/42 (36%)	0/21 (0%)
Sidechain	103/130 (79%)	66/76 (87%)	37/49 (76%)	0/5 (0%)
Aromatic	15/42 (36%)	15/23 (65%)	0/18 (0%)	0/1 (0%)
Overall	175/277 (63%)	123/141 (87%)	52/109 (48%)	0/27 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 63%, i.e. 182 atoms were assigned a chemical shift out of a possible 291. 2 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	58/110 (53%)	43/44 (98%)	15/44 (34%)	0/22 (0%)
Sidechain	109/139 (78%)	70/81 (86%)	39/53 (74%)	0/5 (0%)
Aromatic	15/42 (36%)	15/23 (65%)	0/18 (0%)	0/1 (0%)
Overall	182/291 (63%)	128/148 (86%)	54/115 (47%)	0/28 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

